Chemical Bonds in Dynamics and Microscopy

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Abstract

In many cases, computational chemists use theoretical methods merely as a procedure to compute the potential energy or other property of the system of interest, without paying any attention to the underlying chemical bonding picture. The latter is simply qualitatively assumed, or indeed completely ignored. Indeed, in our group, we often adopt this rather incurious approach in our research. Quite often, though, a higher level of interest towards the nature of bonding can lead to reformulating the problem in such a way that the calculations become more effective, or more insight is obtained.

In this talk, I will describe two examples of such interplay. The first concerns the interpretation and prediction of scanning tunneling microscopy (STM) images for self-assembled monolayers of organic molecules at a surface [1]. A minor change in the structure of the organic molecule – the addition of a methyl group on a saturated alkyl chain – makes a big change to the appearance of the STM image, which can be traced back to the pattern of molecular orbitals in linear and branched alkanes.

The second case concerns the dynamics of cooling of a small molecule after a fast chemical reaction, abstraction of a hydrogen atom from solvent by fluorine atoms [2,3]. The product is initially very highly vibrationally excited, but cools within a few picoseconds, though modelling this is challenging. Insights from bonding suggest various ways to do this.

Reference and notes
